EXHIBIT A

S300

NO

Has a user input a query compound probe?

YES — S310

Create chemical descriptors for the query compound probe.

S320

YES

Has the query compound been modified in view of the ~~created chemical descriptors~~ ranked compounds

NO

S330

Transform the modified query probe into multi-dimensional space using singular value decomposition matrices.

340

Calculate similarity between query probe and compounds database.

S350

Rank compounds by similarity to query probe.

S360

Output a ranked list of compounds

SURESH,
S320 is really not right. We need to talk about this more. Richard
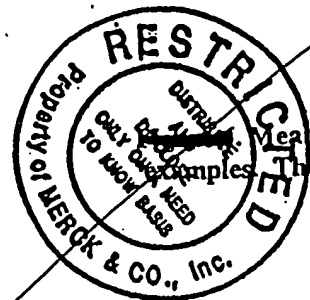
Figure 5

Figure 11

Mean similarity of the probe to each molecule in the top scoring 300 compounds (MSP300) for three examples. The MSP300 for Dice searches are shown as a horizontal lines. For comparison, the MSP300 for random sets of 300 compounds from MDDR would be 0.12-0.14.
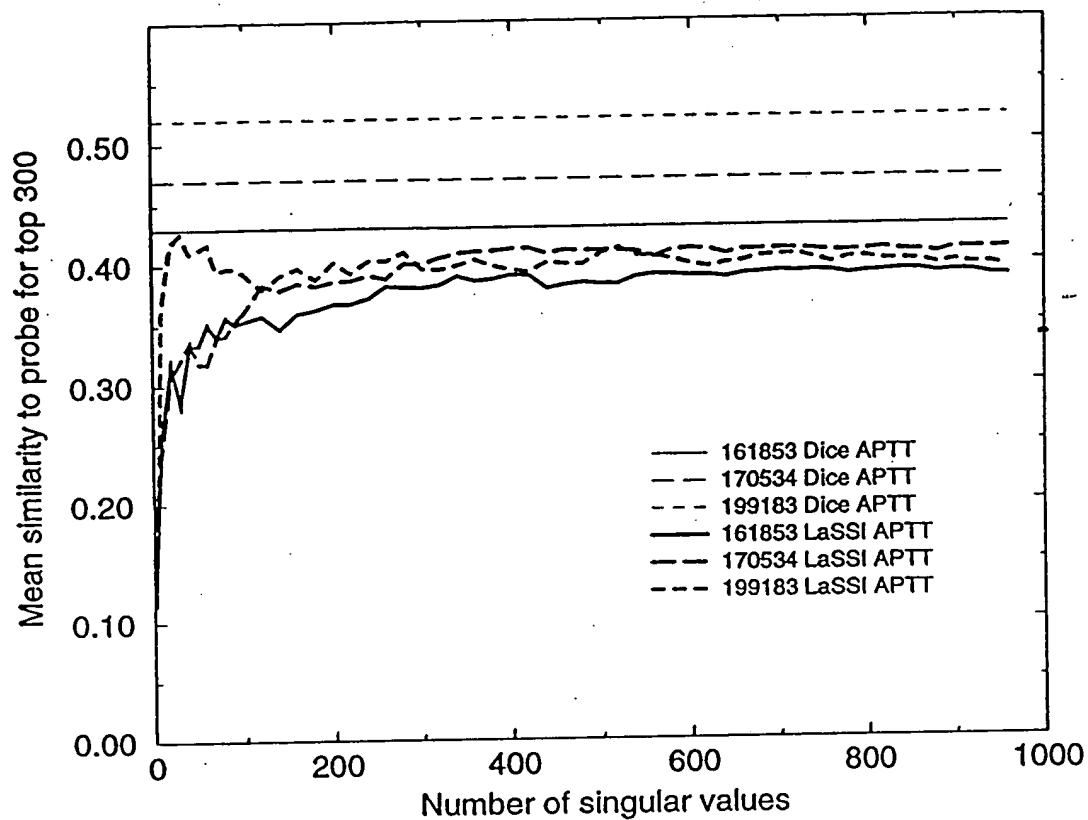
MSP300

Dice TT

Legend:
- 161853 Dice APTT
- 170534 Dice APTT
- 199183 Dice APTT
- 161853 LaSSI APTT
- 170534 LaSSI APTT
- 199183 LaSSI APTT

Y-axis: Mean similarity to probe for top 300
X-axis: Number of singular values

Figure 12

Cumulative actives found vs compounds tested for 187236 as a probe. The actives are oxytocin antagonists that do not contain a dipeptide moiety.

187236 as probe

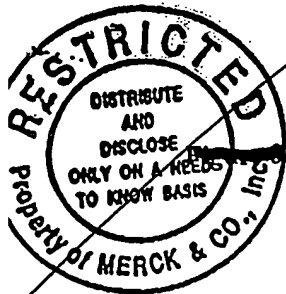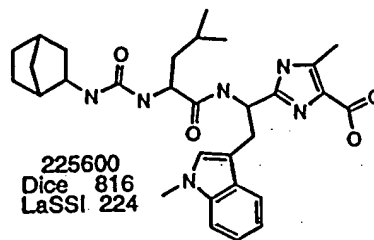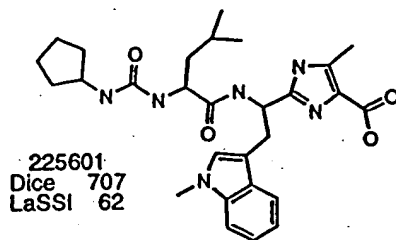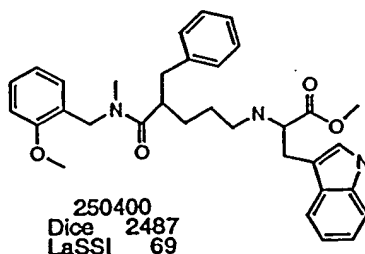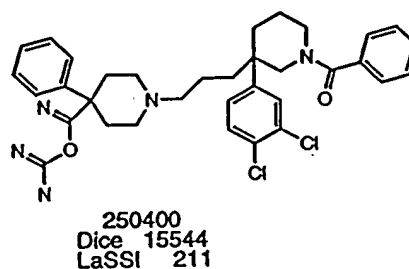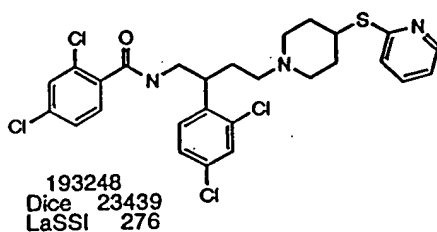### nonpeptide neurokinin antagonists as actives
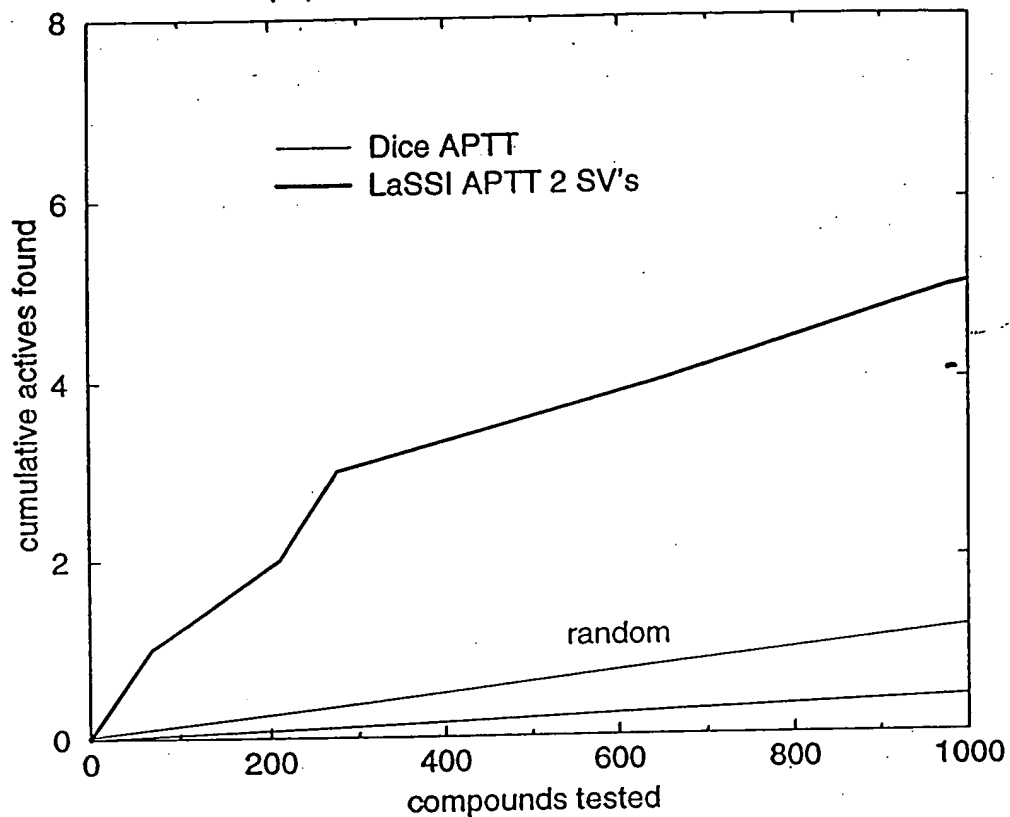
Figure 13

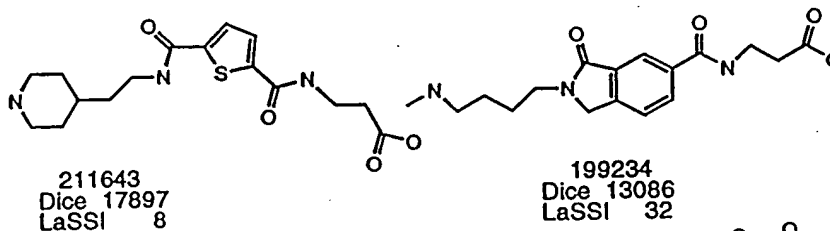Selected non-peptide compounds that have extremely different ranks in Dice APTT vs LaSSI APTT for the statistically significant peptide to non-peptide examples.
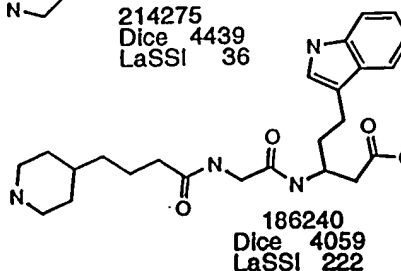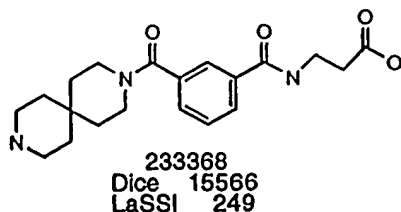
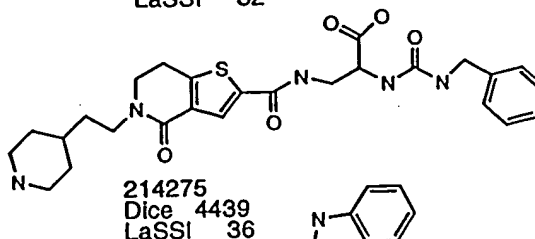174556 endothelin antagonists (9 SV's)

225601
Dice 707
LaSSI 62

225600
Dice 816
LaSSI 224

187236 neurokinin antagonists (2 SV's)

193248
Dice 23439
LaSSI 276

250400
Dice 15544
LaSSI 211

250400
Dice 2487
LaSSI 69

188541 gpIIb/IIIa receptor antagonists (15 SV's)

211643
Dice 17897
LaSSI 8

199234
Dice 13086
LaSSI 32

241493
Dice 11647
LaSSI 82

214275
Dice 4439
LaSSI 36

233368
Dice 15566
LaSSI 249

186240
Dice 4059
LaSSI 222

EXHIBIT   B